Example Based Mini-Course on Mathematical Modelling: Liquid Crystal Transitions

Maha Al hajri, Charles Brett, Andrew Lam

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1   Introduction

In a crystalline solid, the intermolecular forces act on the constituent molecules so that their motion is restricted and they have to lie, on average, in a regular array. When the substance is heated, the molecules gain the necessary kinetic energy to break the crystal structure with large molecular vibrations, leading to a liquid phase.

In certain materials, typically consisting of elongated molecules, the properties are determined by the translational motion and the orientation of the elongated molecules. In an isotropic liquid, the orientation of the molecule is random. However, in the region between the isotropic liquid and crystal states, the orientation of the material is not random, but it exhibits an averaged orientation. *Liquid crystals* are materials which exhibits such orientational order.

One can define a unit vector $\boldsymbol{n}$ as the average molecular orientation direction or the *director*. To measure the amount of orientational order in a small ball $\mathcal{B}$, we can construct a probability distribution of the molecular orientations and look at the mean and variation of the distribution. The usual measure of this variation is via the *scalar order parameter*, denoted by S, defined as the weighted average of the molecular orientation angles θ_m between the long molecular axes and the director:

$$S = \frac{1}{2} \int_{\mathcal{B}} (3\cos^2(\theta_m) - 1) f(\theta_m) dV, \tag{1.1}$$

where $f(\theta_m)$ is the statistical distribution function of the molecular angle θ_m. This function is even and periodic due to the head-tail symmetry of the molecules.

When the material is crystalline and all the molecules align exactly with the director, $\theta_m = 0$ for all molecules and thus $S = 1$. When the material is an isotropic liquid, which means that the molecules are randomly oriented , then $f(\theta_m)$ is a constant and equal to $1/(2\pi)$. Using spherical polar coordinates we find that, after integrating by parts, $S = 0$. We note that when the molecules are randomly oriented in the plane perpendicular to the director, the order parameter is $S = -1/2$ and hence it is possible to achieve a configuration where $-1/2 < S < 0$. But it is more usual that the equilibrium liquid crystal state has a positive order parameter $0 < S < 1$.

Experiments have confirmed the existence of at least three configurations for liquid crystals: a uniaxial configuration (where the molecules are shaped like a cylinder or a rod), a biaxial configuration (where the molecule are rectangular in shape) and the isotropic state.

2 A simple model

Let the director be a non-zero unit vector $\boldsymbol{n}$. Denote $\boldsymbol{n} \otimes \boldsymbol{n}$ as the tensor product of $\boldsymbol{n}$ with itself and define the tensor

$$\boldsymbol{Q} := S(\boldsymbol{n} \otimes \boldsymbol{n} - \frac{1}{3}\boldsymbol{I}), \tag{2.1}$$

where $\boldsymbol{I}$ is the identity tensor. The tensor $\boldsymbol{Q}$ is useful as it is able to characterise the configuration of the material based on the information about its eigenvalues. When $\boldsymbol{Q}$ has three distinct eigenvalues, the configuration is biaxial, when $\boldsymbol{Q}$ has a two degenerate non-zero eigenvalues (i.e. one repeating eigenvalue), the configuration is uniaxial. When $\boldsymbol{Q} = 0$, the configuration is isotropic.

Let $\boldsymbol{\tau}, \boldsymbol{\mu}$ be two vectors such that $(\boldsymbol{n}, \boldsymbol{\tau}, \boldsymbol{\mu})$ forms an orthonormal basis of $\mathbb{R}^3$. Then

$$\boldsymbol{Q}\boldsymbol{n} = S(\boldsymbol{n} - \frac{1}{3}\boldsymbol{n}) = \frac{2}{3}S\boldsymbol{n},$$
$$\boldsymbol{Q}\boldsymbol{\tau} = -\frac{1}{3}S\boldsymbol{\tau},$$
$$\boldsymbol{Q}\boldsymbol{\mu} = -\frac{1}{3}S\boldsymbol{\mu}.$$

Hence the eigenvalues of $\boldsymbol{Q}$ are $\lambda_1 = \frac{2}{3}S$, $\lambda_2 = \lambda_3 = -\frac{1}{3}S$, with corresponding eigenvectors $\boldsymbol{v}_1 = \boldsymbol{n}, \boldsymbol{v}_2 = \boldsymbol{\tau}, \boldsymbol{v}_3 = \boldsymbol{\mu}$. Consequently, the matrix Q has zero trace and is symmetric.

By the theory of symmetric matrices, there exists orthogonal matrix $\boldsymbol{P}$ such that $\boldsymbol{P}^{-1}\boldsymbol{Q}\boldsymbol{P} = \boldsymbol{D}$ where $\boldsymbol{D}$ is the diagonal matrix with $\lambda_1, \lambda_2, \lambda_3$ in its main diagonal. Then for any $k \in \mathbb{N}$, we have

$$\boldsymbol{Q}^k = (\boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{-1})^k = \boldsymbol{P}(\boldsymbol{D})^k\boldsymbol{P}^{-1} \text{ and tr}\left(\boldsymbol{Q}^k\right) = \text{tr}\left(\boldsymbol{P}(\boldsymbol{D})^k\boldsymbol{P}^{-1}\right) = \text{tr}\left(\boldsymbol{D}^k\right) = \sum_{i=1}^{3}\lambda_i^k.$$

We refer the reader to [3] for an introduction to the Q-tensor theory and its applications to liquid crystals.

2.1 Free energy

Within the liquid crystal, there are many forms of energy that make up the total free energy of the material. Examples include the elastic energy of any distortion to the material, the thermotropic energy (that dictates the preferred phase of the material) and the surface energy between the bounding surface and the liquid crystal molecules at the surface. Our main focus in this model is to look for configurations that minimises the thermotropic energy.

From above, we have two degenerate non-zero eigenvalues, hence the equilibrium configurations we expect are the isotropic configuration and the uniaxial configuration. To account for the existence

of two stable minima, we choose the simplest form of the thermotropic energy density, which is the following quartic potential:

$$f(\boldsymbol{Q}(S)) = \frac{A}{2}\operatorname{tr}\left(\boldsymbol{Q}^2\right) - \frac{B}{3}\operatorname{tr}\left(\boldsymbol{Q}^3\right) + \frac{C}{2}\operatorname{tr}\left(\boldsymbol{Q}^4\right), \tag{2.2}$$

where A, B, C are terms that might depend on the temperature of the system. We consider A as a temperature control and we will assume that $B, C > 0$.

Consider a test volume V_c of the crystal and the thermotropic energy in V_c is defined as

$$\begin{aligned}
E(S) &= \int_{V_c} f(\boldsymbol{Q}(S))dV = \int_{V_c} \frac{A}{2}\operatorname{tr}\left(\boldsymbol{Q}^2\right) - \frac{B}{3}\operatorname{tr}\left(\boldsymbol{Q}^3\right) + \frac{C}{2}\operatorname{tr}\left(\boldsymbol{Q}^4\right) dV \\
&= \int_{V_c} \frac{A}{3}S^2 - \frac{2B}{27}S^3 + \frac{C}{9}S^4 dV.
\end{aligned} \tag{2.3}$$

Taking the first variation of $E(S)$ in direction of the function h leads to

$$\begin{aligned}
\lim_{\delta \to 0} \frac{E(S+\delta h) - E(S)}{\delta} &= \lim_{\delta \to 0} \int_{V_c} \frac{1}{\delta}\left(\frac{A}{3}((S+\delta h)^2 - S^2) - \frac{2B}{27}((S+\delta h)^3 - S^3) + \frac{C}{9}((S+\delta h)^4 - S^4)dV\right) \\
&= \int_{V_c} \frac{2A}{3}Sh - \frac{2B}{9}S^2 h + \frac{4C}{9}S^3 h dV.
\end{aligned}$$

Since h is arbitrary, this implies that the minimisers of $E(S)$ satisfy

$$\frac{2A}{3}S - \frac{2B}{9}S^2 + \frac{4C}{9}S^3 = 0. \tag{2.4}$$

Now assume that $\boldsymbol{n}, A, B, C$ are constant and S is time dependent and evolves according to the gradient flow:

$$\int_{V_c} \frac{dS}{dt}hdV = -K \lim_{\delta \to 0} \frac{E(S+\delta h) - E(S)}{\delta},$$

where $K > 0$ is some kinetic rate. Then we have

$$\frac{dS}{dt} = -\frac{2S(t)}{9}(2CS^2 - BS + 3A)K. \tag{2.5}$$

Set $K = 1$ and introduce the following rescaled variables

$$S = \frac{B}{4C}S', \quad A' = \frac{24AC}{B^2}, \quad t' = \frac{36C}{B^2}t$$

we can express (2.5) as

$$\frac{dS'}{dt'} = -S'((S'-1)^2 + A' - 1). \tag{2.6}$$

2.2 Stability analysis of the critical points

The critical points of (2.6) satisfy $\frac{dS'}{dt'} = 0$, and hence we have

- If $A' > 1$, then there is only one critical point: $S' = 0$.

- If $A' = 1$, then there are two critical points: $S' = 0$ and $S' = 1$.

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- If $0 < A' < 1$ and $A' < 0$, then there are three critical points: $S' = 0, S_+, S_-$, where

$$S_\pm = 1 \pm \sqrt{1 - A'}.$$

We denote S_+ as the upper nematic state and S_- as the lower nematic state.

- If $A' = 0$, then there are two critical points: $S' = 0$ and $S' = 2$.

The stability of the critical points of (2.6) can be found using the second derivative

$$\frac{d^2 S'}{d(t')^2} = -3(S')^2 + 4S' - A'.$$

We find that

- If $A' > 1$, then $S' = 0$ is globally stable;

- If $A' = 1'$, then $S' = 0$ is stable and $S' = 1$ is a point of inflection;

- If $0 < A' < 1$, then $S' = 0, S_+$ are stable but $S' = S_-$ is unstable;

- If $A' = 0$, then $S' = 2$ is stable and $S' = 0$ is a point of inflection;

- If $A' < 0$, then $S' = 0$ is unstable and $S' = S_\pm$ are stable.

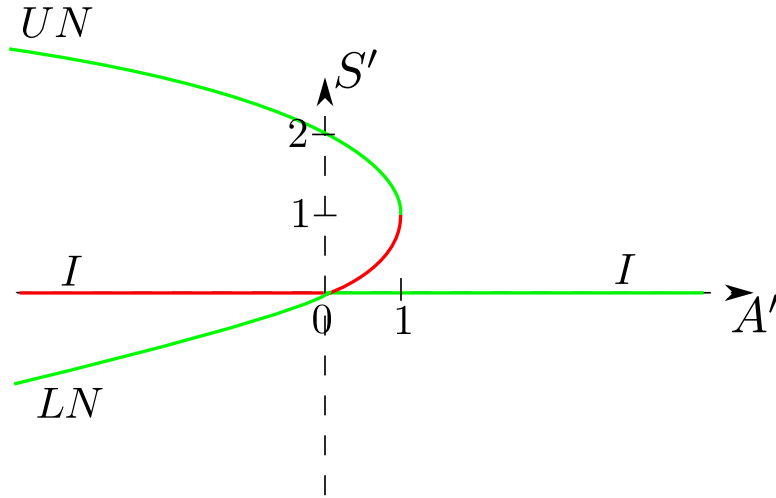This can be summarised in the following response diagram:

Figure 1: Response diagram of the gradient flow with stable (in green) and unstable (in red) critical points.

3   Temperature controlled phase transitions

Suppose we let the temperature vary slowly with time so that

$$A' = A_0 + \varepsilon t', \quad \varepsilon << 1,$$

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where A_0 is some initial temperature. Dropping all the primes and we have

$$\frac{dS}{dt} = -S((S-1)^2 + A_0 + \varepsilon t - 1), \quad S(0) := S_I. \tag{3.1}$$

Then for small ε, we recover (2.6). Hence in the t-timescale, the gradient flow is too fast for us to observe any transition. In the other words, given any initial starting point S_I bounded away from the critical points, (3.1) will only tell us the critical points in which our solution will end up. Thus we need to slow down by rescaling time and set $\tau = \varepsilon t$, leading to

$$\varepsilon\frac{dS}{d\tau} = -S((S-1)^2 + A_0 - 1 + \tau). \tag{3.2}$$

There are three phase transitions we are interested in:

- Transition from Lower Nematic (LN) as temperature increases;

- Transition from Upper Nematic (UN) as temperature increases;
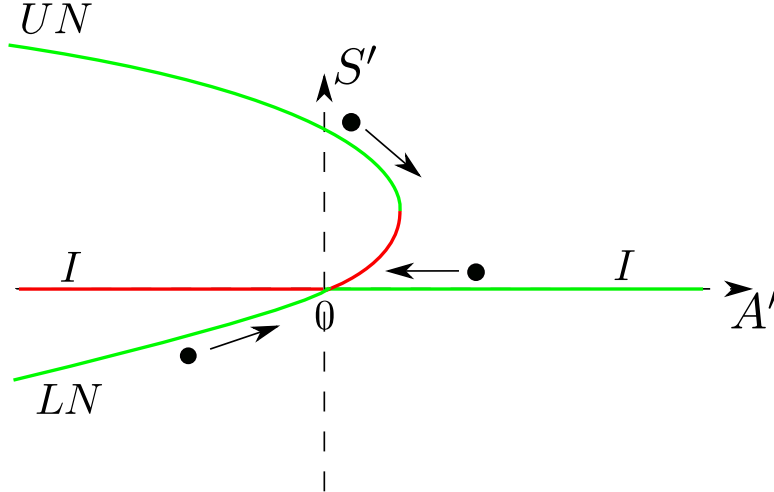
- Transition from Isotropic (I) as temperature decreases;

Figure 2: Phase transitions we will look at

3.1   Forward transition from Lower Nematic

We start near the lower nematic state $S_I \sim S_-$ with $A_0 < 0$. For sufficiently small τ, the equilibria of (3.2) will be only $S = S_-$ if we start close to S_-. One can see this by considering an asymptotic expansion of S:

$$S = S_0 + \varepsilon S_1 + \mathcal{O}(\varepsilon^2). \tag{3.3}$$

Plugging this into (3.2) and matching orders of ε we find that to order $\mathcal{O}(\varepsilon^0)$

$$0 = -S_0(S_0^2 - 2S_0 + (A_0 + \tau)) \tag{3.4}$$

and to order $\mathcal{O}(\varepsilon^1)$

$$\frac{dS_0}{d\tau} = -S_1(3S_0^2 - 4S_0 + (A_0 + \tau)). \tag{3.5}$$

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(3.4) gives the leading term of S as one of the three possible equilibria. Since we started close to S_-, we have that $S_0 = 1 - \sqrt{1 - (A_0 + \tau)}$. Then substitute into (3.5) yields

$$S_1 = -\frac{1}{4([1 - (A_0 + \tau)]^{3/2} - [1 - (A_0 + \tau)])}.$$

Hence we see that the solution S of (3.2) that started close to S_- will look like

$$S = 1 - \sqrt{1 - (A_0 + \tau)} - \frac{\varepsilon}{4([1 - (A_0 + \tau)]^{3/2} - [1 - (A_0 + \tau)])} + \mathcal{O}(\varepsilon^2). \tag{3.6}$$

However, as τ increases to $-A_0$, the two equilibria ($S = 0, S = S_-$) merge into an unstable critical point and it is unclear which critical point the solution will go to. Moreover, the above asymptotic expansion for S no longer holds when $\tau = -A_0$, as the order $\mathcal{O}(\varepsilon)$ term is no longer negligible.

To explore the dynamics near $A = 0$, we perform a formally matched asymptotic analysis. When we are sufficiently away from $A = 0$, we know from above that the solution S is close to S_-. To investigate what happens when A passes through zero, we undergo a rescaling in time and space. This leads to a new differential equation describing the dynamics of the system under the new scales. We now have two ordinary differential equations describing the dynamics for two regions. We expect that in an intermediate region, with A small and negative, the solutions to the two ordinary differential equations should match (see Figure 3).
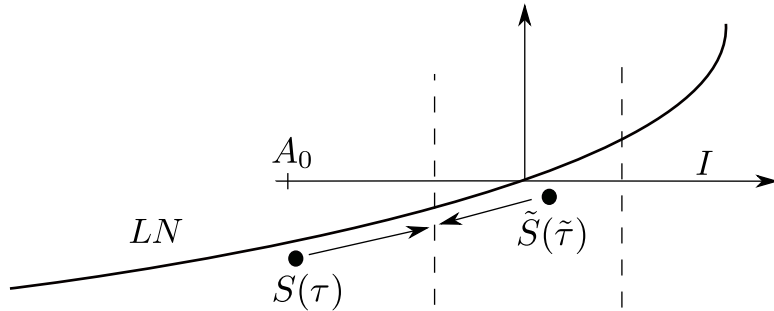

Figure 3: Away from $A = 0$ we have a solution $S(\tau)$ from (3.1) and we have another solution $\tilde{S}(\tilde{\tau})$ in the rescaled (dashed) region close to $A = 0$. The behaviour of both solutions should agree in an intermediate region.

Near the origin $A = 0$, we introduce a new rescaling to zoom in:

$$\tau + A_0 = \varepsilon^\alpha \tilde{\tau}, \quad S = \varepsilon^\beta \tilde{S}, \quad \alpha > 0, \beta > 0.$$

Then substituting these new variables into (3.2) leads to

$$\frac{d\tilde{S}}{d\tilde{\tau}} = -\tilde{S}(\varepsilon^{2\alpha-1}\tilde{\tau} - 2\varepsilon^{\alpha+\beta-1}\tilde{S} + \varepsilon^{\alpha+2\beta-1}\tilde{S}^2) \tag{3.7}$$

To allow for a transition from the lower nematic state under this rescaling, we would like to keep the $\tilde{S}^2$ term and the $\tilde{\tau}\tilde{S}$ term. This requires $2\alpha - 1 = \alpha + \beta - 1 = 1$ and amounts to setting $\alpha = \beta = \frac{1}{2}$. So our rescaled variables are

$$\tau + A_0 = \sqrt{\varepsilon}\tilde{\tau}, \quad S = \sqrt{\varepsilon}\tilde{S}.$$

Then, under this rescaling, (3.2) to least order in ε is

$$\frac{d\tilde{S}}{d\tilde{\tau}} = -\tilde{S}(-2\tilde{S} + \tilde{\tau}). \tag{3.8}$$

The matching condition requires that $\tilde{S}$ matches to the lower nematic state S_- as $\tilde{\tau} \to -\infty$. The equilibria of (3.8) are $\tilde{S} = 0$ corresponding to the isotropic state and $\tilde{S} = \frac{\tilde{\tau}}{2}$ corresponding to the lower nematic state. Hence we need $\tilde{S} \to \frac{\tilde{\tau}}{2}$ as $\tilde{\tau} \to -\infty$.

We observe that (3.8) is a Bernoulli equation. We can substitute $W = \tilde{S}^{-1}$ and solve for $\tilde{S} =: S^I$, the *inner solution*:

$$\tilde{S} = -\exp(-\tilde{\tau}^2/2) \Big/ \left(2\int_{-\infty}^{\tilde{\tau}} \exp(-\eta^2/2)d\eta\right). \tag{3.9}$$

We note that $\tilde{S} \to 0$ as $\tilde{\tau} \to +\infty$ at an exponential rate. In other words, we have switched from the lower nematic state to the isotropic state on a timescale $\tau = \mathcal{O}(\sqrt{\varepsilon})$ or $t = \mathcal{O}(1/\sqrt{\varepsilon})$.

3.2 Forward transition from Upper Nematic

We start near the upper nematic state $S_I \sim S_+$ with $A_0 < 1$. With the same asymptotic expansion (3.3), we see that the solution S can be expressed as

$$S = 1 + \sqrt{1 - (A_0 + \tau)} + \frac{\varepsilon}{4([1 - (A_0 + \tau)]^{3/2} + [1 - (A_0 + \tau)])} + \mathcal{O}(\varepsilon^2).$$

This expansion breaks down when $A_0 + \tau$ approaches 1 and so we consider the following rescaling to explore the dynamics near $A = 1$:

$$\tau + A_0 - 1 = \varepsilon^\alpha \tilde{\tau}, \quad S - 1 = \varepsilon^\beta \tilde{S},$$

then we have

$$\frac{d\tilde{S}}{d\tilde{\tau}} = -\varepsilon^{\beta+\alpha-1}\tilde{S}^2 - \varepsilon^{2\alpha-\beta-1}\tilde{\tau} - \varepsilon^{2\beta+\alpha-1}\tilde{S}^3 - \varepsilon^{2\alpha-1}\tilde{\tau}\tilde{S}.$$

We choose $\alpha = \frac{2}{3}$ and $\beta = \frac{1}{3}$ to obtain, to lowest order of ε:

$$\frac{d\tilde{S}}{d\tilde{\tau}} = -(\tilde{S}^2 + \tilde{\tau}). \tag{3.10}$$

(3.10) is a Riccati equation and we use the ansatz $\tilde{S} = u'/u$ for some function u to obtain the following Airy equation:

$$\frac{d^2u}{d\tilde{\tau}^2} + \tilde{\tau}u = 0. \tag{3.11}$$

The solution to (3.11) is

$$u(\tilde{\tau}) = C_1 \mathrm{Ai}(-\tilde{\tau}) + C_2 \mathrm{Bi}(-\tilde{\tau}), \tag{3.12}$$

where C_1, C_2 are constants and

$$\mathrm{Ai}(x) = \frac{1}{\pi}\int_0^\infty \cos(\tfrac{1}{3}t^3 + xt)dt, \quad \mathrm{Bi}(x) = \frac{1}{\pi}\int_0^\infty [\exp(-\tfrac{1}{3}t^3 + xt) + \sin(\tfrac{1}{3}t^3 + xt)]dt$$
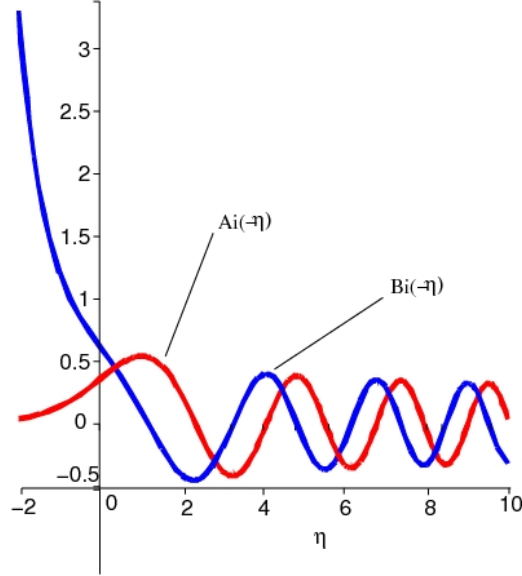
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Figure 4: Plots of $\mathrm{Ai}(-\eta)$ and $\mathrm{Bi}(-\eta)$.

are the Airy functions of the first and second kind. We choose $C_1 = 1$ and $C_2 = 0$ to give

$$\tilde{S}(\tilde{\tau}) = \frac{-\mathrm{Ai}'(-\tilde{\tau})}{\mathrm{Ai}(-\tilde{\tau})}. \tag{3.13}$$

We refer to [1] (pages 448–449) for the asymptotic formulae for $\mathrm{Ai}(z), \mathrm{Ai}'(z)$ for $|z|$ large. For $\tilde{\tau}$ large and negative, the solution $\tilde{S}$ behaves like

$$\tilde{S}(\tilde{\tau}) \sim \sqrt{-\tilde{\tau}}, \qquad \text{as } \tilde{\tau} \to -\infty,$$

which matches with the upper nematic state as $\tilde{\tau} \to -\infty$. We observe that (3.13) is valid until $\tilde{\tau} = \tau^*$, where $-\tau^*$ is the first zero of the Airy function ($\tau^* \approx +2.338$). This motivates us to look at $A = 1 + \varepsilon^{2/3}\tau^* + \varepsilon\tilde{\tau}$, then we have

$$\frac{d\tilde{S}}{d\tilde{\tau}} = -\tilde{S}((\tilde{S} - 1)^2 + \tau^*\varepsilon^{2/3} + \varepsilon\tilde{\tau})$$

and to lowest order we obtain

$$\frac{d\tilde{S}}{d\tilde{\tau}} = -\tilde{S}(\tilde{S} - 1)^2.$$

Using separation of variables, we arrive at the implicit solution

$$\tilde{\tau} \sim -\frac{1}{1 - \tilde{S}} + \log\left(\frac{1 - \tilde{S}}{\tilde{S}}\right).$$

As $\tilde{\tau} \to +\infty$ we must have $\tilde{S} \to 0$. Hence we observed a transition from the upper nematic state to the isotropic state on a timescale of $\tau = \mathcal{O}(\varepsilon^{2/3})$.

3.3 Backward transition from Isotropic

Starting with S_I arbitrary but small (so that the dynamics of (3.1) will drive it to the isotropic state) and $0 < A_0 < 1$. We want to investigate the transition from the isotropic state when we bring the

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temperature down. We consider $A = A_0 - \tau, \tau = \varepsilon t$ and look at the following rescaling

$$\tau = \varepsilon^\alpha \tilde\tau, \quad S = \varepsilon^\beta \tilde S.$$

Here we have decided not to include A_0 into the rescaling of τ as we also want to investigate the effects of A_0 on the transition. Substituting these into (3.2) yields

$$\frac{d\tilde S}{d\tilde\tau} = -\tilde S(\varepsilon^{2\beta+\alpha-1}\tilde S^2 - 2\varepsilon^{\beta+\alpha-1}\tilde S + A_0\varepsilon^{\alpha-1} - \tilde\tau\varepsilon^{2\alpha-1}).$$

From the earlier stability analysis (Section 2.2), we know that the isotropic state is stable for $A > 0$, this motivates us to keep the last two terms and discard the first two terms. Then the resulting ODE will only have a critical point at $\tilde S = 0$. However, there is no value of α such that $\alpha - 1$ and $2\alpha - 1$ can both equal to zero. Hence we set $\alpha = 0$ and $\beta > 1$ and look at the resulting ODE up to order $\mathcal{O}(1)$, which is

$$\frac{d\tilde S}{d\tilde\tau} = \tilde S\left(\frac{\tilde\tau - A_0}{\varepsilon}\right).$$

This yields a solution

$$\tilde S(\tilde\tau) = \tilde S(0) \exp\left(\frac{\tilde\tau^2}{2\varepsilon} - \frac{A_0\tilde\tau}{\varepsilon}\right)$$

and we observe the following:

$$\begin{cases} \tilde S \sim 0, & \text{if } 0 < \tilde\tau < 2A_0, \\ \tilde S \to +\infty, & \text{if } \tilde\tau \to \infty, \tilde S(0) > 0, \\ \tilde S \to -\infty, & \text{if } \tilde\tau \to \infty, \tilde S(0) < 0. \end{cases}$$

So, once $\tilde\tau$ goes above $2A_0$, or equivalently, A goes below $-A_0$, $\tilde S$ either jumps up to $+\infty$ or jumps to $-\infty$ depending on the sign of $\tilde S(0)$.

4 Conclusion and Future research

In this report, we have derived a simple model for the dynamics of liquid crystals via Q-tensor theory, which avoids the problems of angle representation. Instead, the variation in orientation of the molecules in the liquid crystal is summarised by the scalar order parameter S. Applying a gradient flow to the thermotropic energy, which we take as a quartic potential, we derived an ordinary differential equation for S, and analysed the stability of its critical points. Moreover, we use the method of formally matched asymptotics to formally deduce the phase transitions from one equilibrium state to another when the temperature is varied. Our main results are summarised in Figure 5. Namely the forward transitions from nematic states to isotropic state as the temperature increases. However, we observed a delayed bifurcation for the backward transition from the isotropic state, where the order parameter S' stayed close to zero for values of A' where the isotropic state is unstable.

In our model, we only considered the case where the director $\boldsymbol{n}$ and the scalar order parameter S are spatially independent. One could have considered the following spatially varying energy functional
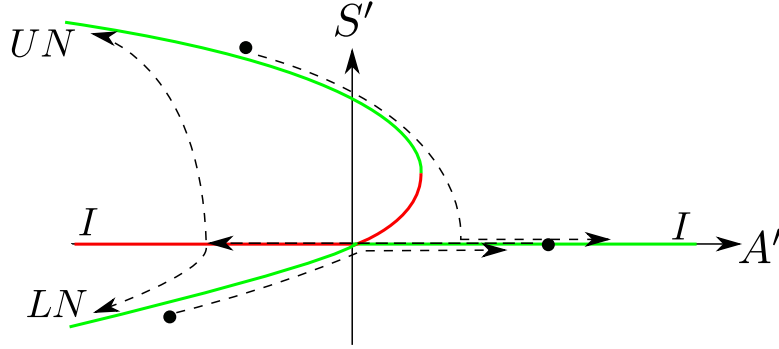
Figure 5: Full response diagram with phase transitions.

as opposed to (2.3):

$$E_1 = \int_{V_c} \frac{\eta}{2} |\nabla S|^2 + f(\boldsymbol{Q}(S)), \tag{4.1}$$

where $\eta > 0$ is some constant. The gradient flow of this energy would then lead to the following partial differential equation:

$$\partial_t S = \eta \nabla^2 S - \frac{2S}{9}(2CS^2 - BS + 3A(T(\boldsymbol{x}, t)), \tag{4.2}$$

where $T(\boldsymbol{x}, t)$ is the temperature. The one-dimensional version of the above PDE have been considered in [2]. Another possible research direction is to extend the energy E to include the electromagnetic energy and the surface energy as done in [3]. A third direction is to consider the phase transitions in the context of optimal control and inverse problems, i.e. what is the temperature control is needed for a desired pattern of phases.

References

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